```
=> fil casreact
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                               0.21       0.21

FILE 'CASREACT' ENTERED AT 16:05:53 ON 15 NOV 2005
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FILE CONTENT:1840 - 13 Nov 2005 VOL 143 ISS 20

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*************************************************************
*                                                           *
*     CASREACT now has more than 9.2 million reactions      *
*                                                           *
*************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10785627\rxn1.str
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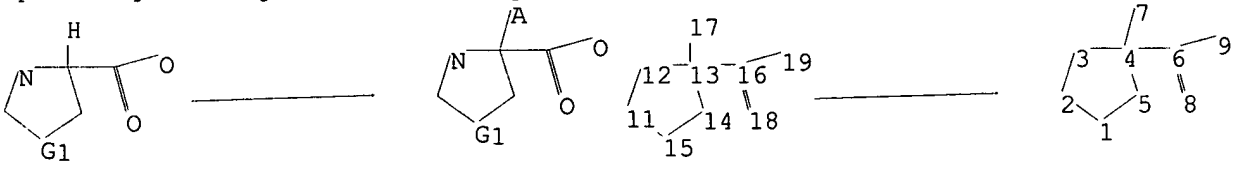


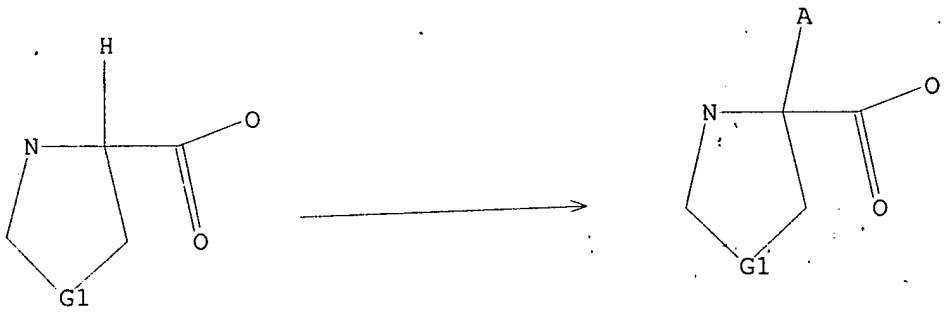

```
chain nodes :
6  7  8  9  16  17  18  19
ring nodes :
1  2  3  4  5  11  12  13  14  15
chain bonds :
4-6  4-7  6-8  6-9  13-16  13-17  16-18  16-19
ring bonds :
1-2  1-5  2-3  3-4  4-5  11-12  11-15  12-13  13-14  14-15
exact/norm bonds :
1-2  1-5  2-3  3-4  4-5  4-6  4-7  6-8  6-9  11-12  11-15  12-13  13-14  13-16
13-17  14-15  16-18  16-19
isolated ring systems :
containing 1 : 11 :
```

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 11
node mappings:
4:13 6:16 5:14 2:11 3:12

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 16:06:24 FILE 'CASREACT'
SCREENING COMPLETE - 2012 REACTIONS TO VERIFY FROM 156 DOCUMENTS

100.0% DONE 2012 VERIFIED 5 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 37555 TO 42925
PROJECTED ANSWERS: 1 TO 79

L2 1 SEA SSS SAM L1 (5 REACTIONS)

=> s l1 full
FULL SEARCH INITIATED 16:06:35 FILE 'CASREACT'
SCREENING COMPLETE - 43189 REACTIONS TO VERIFY FROM 2748 DOCUMENTS

100.0% DONE 43189 VERIFIED 75 HIT RXNS 17 DOCS
SEARCH TIME: 00.00.03

L3 17 SEA SSS FUL L1 (75 REACTIONS)

=> d ibib 1-17

L3 ANSWER 1 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 142:6783 CASREACT
TITLE: Stereocontrolled α-alkylation of fully protected L-serine
AUTHOR(S): Brunner, Martin; Saarenketo, Pauli; Straub, Thomas; Rissanen, Kari; Koskinen, Ari M. P.
CORPORATE SOURCE: Laboratory of Organic Chemistry, Helsinki University of Technology, Espoo, 02150, Finland
SOURCE: European Journal of Organic Chemistry (2004), (18), 3879-3883
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 141:243544 CASREACT
TITLE: Process for electrophilic substitution of thiazolidinecarboxylates or oxazolidinecarboxylates
INVENTOR(S): Heldmann, Dieter; Stohrer, Juergen
PATENT ASSIGNEE(S): Consortium fuer Elektrochemische Industrie G.m.b.H., Germany
SOURCE: Eur. Pat. Appl., 17 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1452529	A1	20040901	EP 2004-3742	20040219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
DE 10308580	B3	20040909	DE 2003-10308580	20030227
US 2004171840	A1	20040902	US 2004-785627	20040224
PRIORITY APPLN. INFO.:			DE 2003-10308580	20030227

OTHER SOURCE(S): MARPAT 141:243544
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 141:7410 CASREACT
TITLE: Highly diastereoselective aldol additions to five-ring N,O-acetals
AUTHOR(S): Brunner, Martin; Koskinen, Ari M. P.
CORPORATE SOURCE: Laboratory of Organic Chemistry, Helsinki University of Technology, Espoo, FIN-02150, Finland
SOURCE: Tetrahedron Letters (2004), 45(15), 3063-3065
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal

LANGUAGE: English
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 138:304273 CASREACT
TITLE: Preparation of 2-aryl-4-methylthiazol-(4S)-carboxylic acids via the condensation of 2-methyl-D-cysteine and arylnitriles
INVENTOR(S): Krich, Sylvia; Rieder, Alexander; Heu, Ferdinand; Steinbauer, Gerhard
PATENT ASSIGNEE(S): DSM Fine Chemicals Austria NFG GmbH & Co. KG, Austria
SOURCE: Eur. Pat. Appl., 13 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1302467	A2	20030416	EP 2002-21002	20020920
EP 1302467	A3	20030502		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2003088105	A1	20030508	US 2002-270324	20021015
US 6894170	B2	20050517		
JP 2003201284	A2	20030718	JP 2002-300807	20021015
US 2005101782	A1	20050512	US 2004-11110	20041215
PRIORITY APPLN. INFO.:			AT 2001-1639	20011016
			US 2002-270324	20021015

OTHER SOURCE(S): MARPAT 138:304273

L3 ANSWER 5 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 138:39490 CASREACT
TITLE: Stereoselective synthesis of amino-substituted apio dideoxynucleosides through a distant neighboring group effect
AUTHOR(S): Choi, Won Jun; Ahn, Hee Sung; Kim, Hea Ok; Kim, Sanghee; Chun, Moon Woo; Jeong, Lak Shin
CORPORATE SOURCE: College of Pharmacy, Laboratory of Medicinal Chemistry, Ewha Womans University, Seoul, 120-750, S. Korea
SOURCE: Tetrahedron Letters (2002), 43(35), 6241-6243
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 137:279432 CASREACT
TITLE: Electrolytic partial fluorination of organic compounds. Part 61: The first example of direct α-fluorination of protected α-amino acids
AUTHOR(S): Baba, Daisuke; Fuchigami, Toshio

CORPORATE SOURCE: Department of Electronic Chemistry, Tokyo Institute of Technology, Nagatsuta, Midori-ku, Yokohama, 226-8502, Japan
SOURCE: Tetrahedron Letters (2002); 43(27), 4805-4808
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 137:181472 CASREACT
TITLE: Alpha-alkylcysteines as inhibitors for carboxypeptidase A. Synthesis, evaluation, and implication for inhibitor design strategy
AUTHOR(S): Lee, Hyun Soo; Kim, Dong H.
CORPORATE SOURCE: Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (2002), 23(4), 593-598
CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 136:151019 CASREACT
TITLE: Synthetic studies toward kaitocephalin
AUTHOR(S): Loh, T.-P.; Chok, Y.-K.; Yin, Z.
CORPORATE SOURCE: Department of Chemistry, National University of Singapore, Singapore, 117543, Singapore
SOURCE: Tetrahedron Letters (2001), 42(44), 7893-7897
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 9 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 135:5516 CASREACT
TITLE: Asymmetric synthesis of quaternary tetrahydroisoquinoline-3-carboxylic acid derivatives
AUTHOR(S): Alezra, V.; Bonin, M.; Micouin, L.; Husson, H.-P.
CORPORATE SOURCE: Faculte des Sciences Pharmaceutiques et Biologiques, Laboratoire de Chimie Therapeutique associe au CNRS et a l'Universite Rene Descartes, Paris, 75270, Fr.
SOURCE: Tetrahedron Letters (2001), 42(11), 2111-2113
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 133:17760 CASREACT
TITLE: Asymmetric functionalization of a chiral non-racemic oxazolidine ester enolate. A new route towards the preparation of quaternary serine esters
AUTHOR(S): Alezra, Valerie; Bonin, Martine; Chiaroni, Angele; Micouin, Laurent; Riche, Claude; Husson, Henri-Philippe
CORPORATE SOURCE: Laboratoire de Chimie Therapeutique associe au CNRS et a l'Universite Rene Descartes (UMR 8638), Faculte des Sciences Pharmaceutiques et Biologiques, Paris, 75270, Fr.
SOURCE: Tetrahedron Letters (2000), 41(11), 1737-1740
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 119:73043 CASREACT
TITLE: Enantioselective synthesis of 2-alkyl substituted cysteines
AUTHOR(S): Pattenden, Gerald; Thom, Stephen M.; Jones, Martin F.
CORPORATE SOURCE: Dep. Chem., Univ. Nottingham, Nottingham, NG7 2RD, UK
SOURCE: Tetrahedron (1993), 49(10), 2131-8
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English

L3 ANSWER 12 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 118:60072 CASREACT
TITLE: Total synthesis of lactacystin
AUTHOR(S): Corey, E. J.; Reichard, Gregory A.
CORPORATE SOURCE: Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA
SOURCE: Journal of the American Chemical Society (1992), 114(26), 10677-8
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

L3 ANSWER 13 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 114:24532 CASREACT
TITLE: Synthesis of 2-carboxy-substituted sphingosine derivatives
AUTHOR(S): Singh, Narrinder P.; Giannis, Athanassios; Henk, Elfi; Kolter, Thomas; Sandhoff, Konrad; Schmidt, Richard R.
CORPORATE SOURCE: Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Germany
SOURCE: Journal of Carbohydrate Chemistry (1990), 9(5), 543-59
CODEN: JCACDM; ISSN: 0732-8303
DOCUMENT TYPE: Journal
LANGUAGE: English

L3 ANSWER 14 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 108:187232 CASREACT
TITLE: Stereoselective alkylation at C(α) of serine, glyceric acid, threonine, and tartaric acid involving heterocyclic enolates with exocyclic double bonds
AUTHOR(S): Seebach, Dieter; Aebi, Johannes D.; Gander-Coquoz, Marlyse; Naef, Reto
CORPORATE SOURCE: Lab. Org. Chem., Eidg. Tech. Hochsch., Zurich, CH-8092, Switz.
SOURCE: Helvetica Chimica Acta (1987), 70(4), 1194-216
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German

IDS

L3 ANSWER 15 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 105:133326 CASREACT
TITLE: Asymmetric Michael additions. Stereoselective alkylation of chiral, non-racemic enolates by nitro olefins. Preparation of enantiomerically pure γ-aminobutyric and succinic acid derivatives
AUTHOR(S): Calderari, Giorgio; Seebach, Dieter
CORPORATE SOURCE: Lab. Org. Chem., Eidg. Tech. Hochsch., Zurich, CH-8092, Switz.
SOURCE: Helvetica Chimica Acta (1985), 68(6), 1592-604
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German

Not online

Q01.HW

L3 ANSWER 16 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 101:230964 CASREACT
TITLE: α-Alkylation of serine with self-reproduction of the center of chirality
AUTHOR(S): Seebach, Dieter; Aebi, Johannes D.
CORPORATE SOURCE: Lab. Org. Chem., Eidg. Tech. Hochsch., Zurich, CH-8092, Switz.
SOURCE: Tetrahedron Letters (1984), 25(24), 2545-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English

IDS

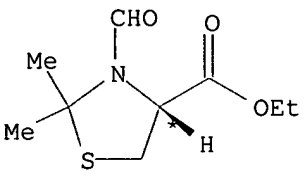
L3 ANSWER 17 OF 17 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 86:5357 CASREACT
TITLE: Metalated nitrogen derivatives of carbonic acid in organic synthesis, VIII. 2-Thioxo-oxazolidines by cycloaddition of α-metalated alkyl isothiocyanates to carbonyl compounds
AUTHOR(S): Hoppe, Dieter; Follmann, Rainer
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Goettingen, Goettingen, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1976), 109(9), 3047-61
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German

=> d hit 4-17

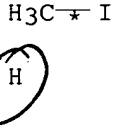
4

L3 ANSWER 4 OF 17 CASREACT COPYRIGHT 2005 ACS on STN

RX(9) OF 48 ...**W** + H ===> **Y**...



W



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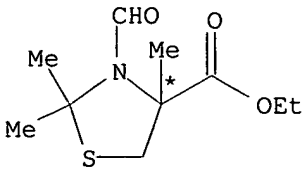


Y

RX(9) RCT W **511303-27-8**

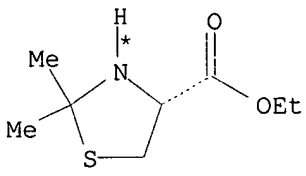
STAGE(1)
RGT K 4111-54-0 LiN(Pr-i)2
SOL 1634-04-4 t-BuOMe
CON 20 minutes, -50 deg C

STAGE(2)
RCT H 74-88-4
SOL 7226-23-5 DMPU
CON 1.5 hours, -50 deg C

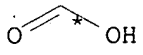
PRO Y **511303-30-3**

LDA
t-BuOMe / DMPU
-50 °C

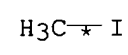
RX(20) OF 48 COMPOSED OF RX(8), RX(9)
RX(20) **U** + V + H ===> **Y**



U

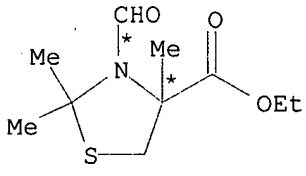


V



H

2 STEPS



Y

RX(8) RCT U **64331-72-2**, V 64-18-6
PRO W 511303-27-8
SOL 108-24-7 Ac2O

CON 1 hour, reflux
NTE stereoselective

RX(9) RCT W 511303-27-8

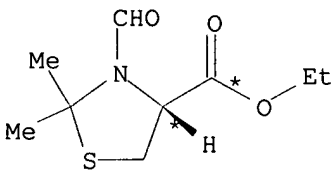
STAGE(1)
RGT K 4111-54-0 LiN(Pr-i)2
SOL 1634-04-4 t-BuOMe
CON 20 minutes, -50 deg C

STAGE(2)
RCT H 74-88-4
SOL 7226-23-5 DMPU
CON 1.5 hours, -50 deg C

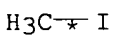
PRO Y **511303-30-3**

-50 °C

RX(21) OF 48 COMPOSED OF RX(9), RX(10)
RX(21) **W** + H ===> **E**

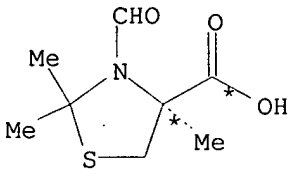


W



H

2 STEPS



E
YIELD 80%

RX(9) RCT W **511303-27-8**

STAGE(1)
RGT K 4111-54-0 LiN(Pr-i)2
SOL 1634-04-4 t-BuOMe
CON 20 minutes, -50 deg C

STAGE(2)
RCT H 74-88-4
SOL 7226-23-5 DMPU
CON 1.5 hours, -50 deg C

PRO Y 511303-30-3

RX(10) RCT Y 511303-30-3

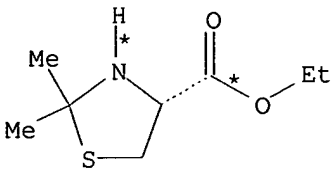
STAGE(1)
SOL 68-12-2 DMF, 7732-18-5 Water
CON 7 minutes, room temperature

STAGE(2)
RGT AA 7558-80-7 NaH2PO4
CON 24 hours, room temperature

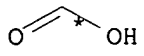
R.T.

PRO E **511303-33-6**
NTE biotransformation, buffered soln., enzymic, stereoselective

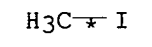
RX(34) OF 48 COMPOSED OF RX(8), RX(9), RX(10)
RX(34) **U** + V + H ===> **E**



U

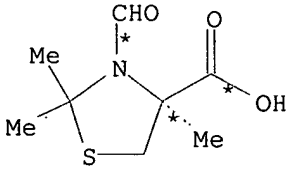


V



H

3 STEPS



E
YIELD 80%

RX(8) RCT U **64331-72-2**, V 64-18-6
PRO W 511303-27-8
SOL 108-24-7 Ac2O
CON 1 hour, reflux
NTE stereoselective

RX(9) RCT W 511303-27-8

STAGE(1)
RGT K 4111-54-0 LiN(Pr-i)2
SOL 1634-04-4 t-BuOMe
CON 20 minutes, -50 deg C

STAGE(2)
RCT H 74-88-4
SOL 7226-23-5 DMPU
CON 1.5 hours, -50 deg C

PRO Y 511303-30-3

RX(10) RCT Y 511303-30-3

STAGE(1)
SOL 68-12-2 DMF, 7732-18-5 Water
CON 7 minutes, room temperature

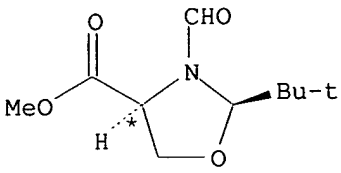
STAGE(2)
RGT AA 7558-80-7 NaH2PO4
CON 24 hours, room temperature

PRO E **511303-33-6**
NTE biotransformation, buffered soln., enzymic, stereoselective

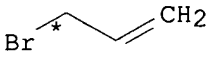
5

L3 ANSWER 5 OF 17 CASREACT COPYRIGHT 2005 ACS on STN

RX(1) OF 70 **A** + B ===> **C**...

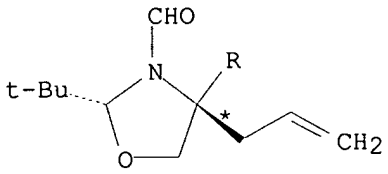


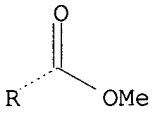
A



B

(1) →





C
YIELD 55%

RX(1) RCT A **93250-91-0**, B 106-95-6
RGT D 4111-54-0 LiN(Pr-i)2, E 680-31-9 HMPT
PRO C **93250-96-5**
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

X

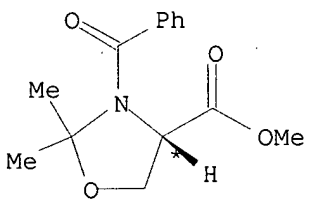
-78°C

— Electrochemistry

6

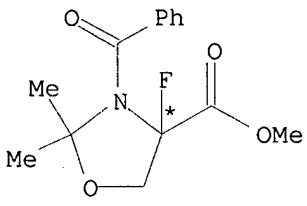
L3 ANSWER 6 OF 17 CASREACT COPYRIGHT 2005 ACS on STN

RX(1) OF 3 **A** ===> **B**



A

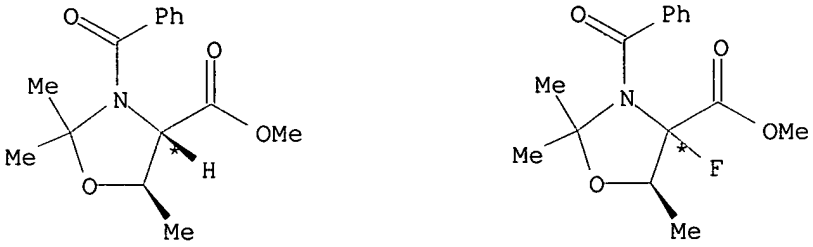
(1) →



B
YIELD 66%

RX(1) RCT A **467233-08-5**
RGT C 665-46-3 Et4N.F, D 7664-39-3 HF
PRO B **467233-11-0**
CAT 7440-06-4 Pt
SOL 75-05-8 MeCN
NTE Electrochem., platinum anode, alternative reaction conditions gave lower yield

RX(2) OF 3 **G** ===> **H**

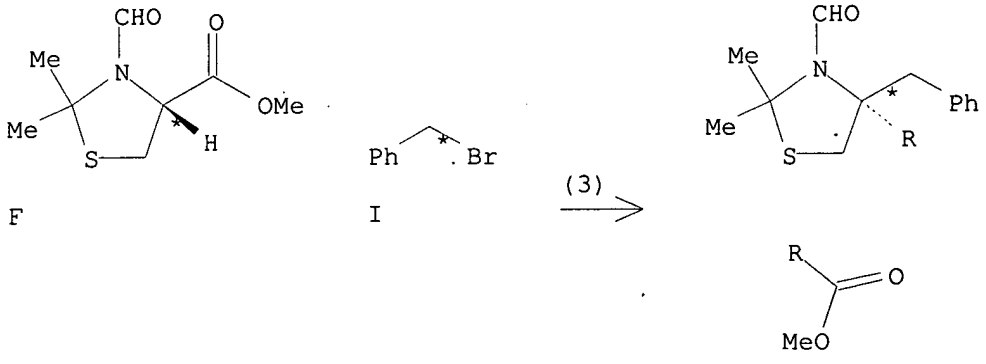


G (2) H
YIELD 73%

RX(2) RCT G **467233-09-6**
RGT C 665-46-3 Et4N.F, D 7664-39-3 HF
PRO H **467233-12-1**
CAT 7440-06-4 Pt
SOL 75-05-8 MeCN
NTE Electrochem., platinum anode, alternative reaction conditions gave lower yield, stereoselective

L3 ANSWER 7 OF 17 CASREACT COPYRIGHT 2005 ACS on STN

RX(3) OF 46 ...**F** + I ===> **J**...



F I (3)

J
YIELD 30%

RX(3) RCT F **62972-76-3**

STAGE(1)
RGT K 7226-23-5 DMPU, L 109-72-8 BuLi, M 108-18-9 i-Pr2NH
SOL 109-99-9 THF, 110-54-3 Hexane

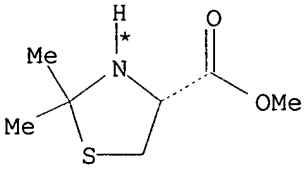
STAGE(2)
RCT I 100-39-0

PRO J **450359-14-5**

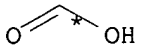
LDA DMPU
THF, Hex

2.

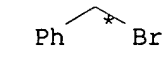
RX(14) OF 46 COMPOSED OF RX(2), RX(3)
RX(14) **C** + E + I ===> **J**



C

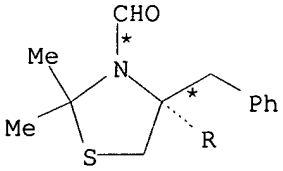


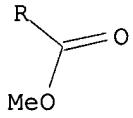
E



I

2 STEPS





J
YIELD 30%

RX(2) RCT C **19907-59-6**, E 64-18-6
RGT G 108-24-7 Ac2O, H 141-53-7 Na formate
PRO F 62972-76-3

RX(3) RCT F 62972-76-3

STAGE(1)
RGT K 7226-23-5 DMPU, L 109-72-8 BuLi, M 108-18-9 i-Pr2NH
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)
RCT I 100-39-0

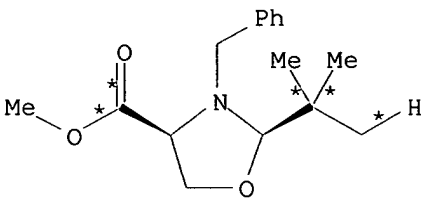
PRO J **450359-14-5**

LDA
DMPU/THF/
Hex

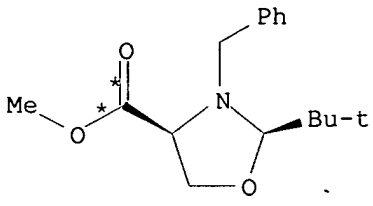
8

L3 ANSWER 8 OF 17 CASREACT COPYRIGHT 2005 ACS on STN

RX(26) OF 61 COMPOSED OF RX(3), RX(4), RX(5)
RX(26) 2 **H** ===> **Q**

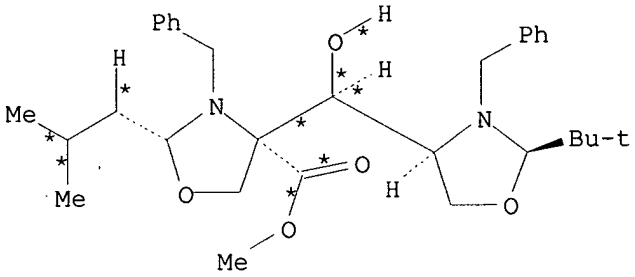


H



H

3 STEPS



Q
YIELD 51%

RX(3) RCT H **145451-89-4**
RGT E 16940-66-2 NaBH4
PRO K 393867-18-0
SOL 67-56-1 MeOH, 109-99-9 THF

RX(4) RCT K 393867-18-0

STAGE(1)
RGT N 79-37-8 (COCl)2, O 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT D 121-44-8 Et3N

PRO M 393867-20-4
NTE Swern oxidn.

RX(5) RCT H **145451-89-4**

STAGE(1)
RGT R 4039-32-1 (Me3Si)2N.Li
SOL 109-99-9 THF

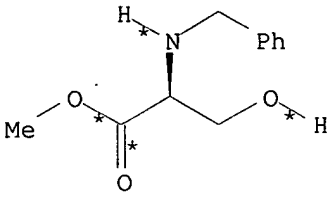
HMDS

STAGE(2)

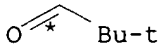
RCT M 393867-20-4

PRO Q **393867-22-6**
NTE stereoselective, optimization study, optimized on base,additives,time

RX(29) OF 61 COMPOSED OF REACTION SEQUENCE RX(2), RX(5) AND REACTION SEQUENCE RX(3), RX(4), RX(5)
...C + G ===> H...
...2 **H** ===> **Q**

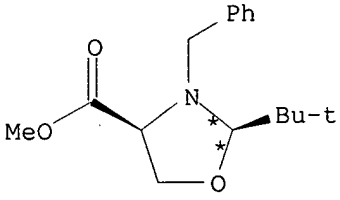


C



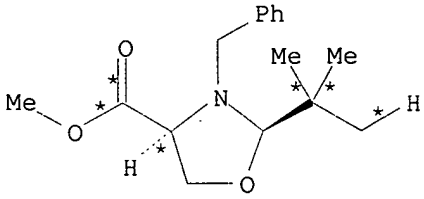
G

3 STEPS

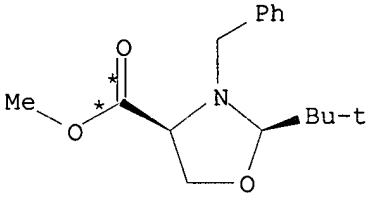


H

START NEXT REACTION SEQUENCE

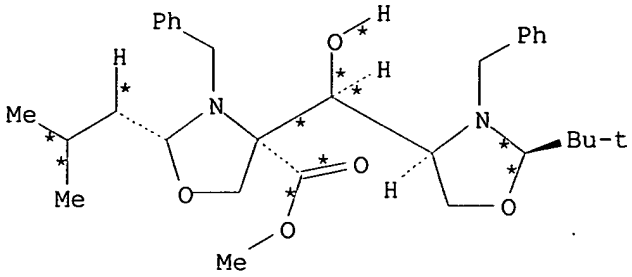


H



H

3 STEPS



Q
YIELD 51%

RX(2) RCT C 123639-56-5, G 630-19-3
PRO H 145451-89-4
CAT 104-15-4 TsOH
SOL 108-88-3 PhMe
NTE stereoselective

RX(3) RCT H **145451-89-4**
RGT E 16940-66-2 NaBH4
PRO K 393867-18-0
SOL 67-56-1 MeOH, 109-99-9 THF

RX(4) RCT K 393867-18-0

STAGE(1)
RGT N 79-37-8 (COCl)2, O 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT D 121-44-8 Et3N

PRO M 393867-20-4
NTE Swern oxidn.

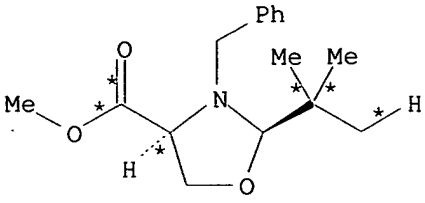
RX(5) RCT H **145451-89-4**

STAGE(1)
RGT R 4039-32-1 (Me3Si)2N.Li
SOL 109-99-9 THF

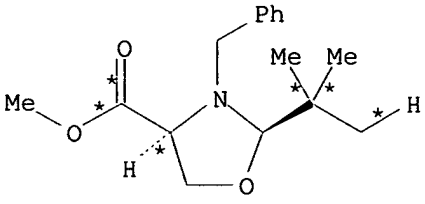
STAGE(2)
RCT M 393867-20-4

PRO Q **393867-22-6**
NTE stereoselective, optimization study, optimized on base,additives,time

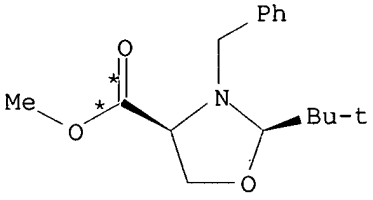
RX(30) OF 61 COMPOSED OF RX(3), RX(4), RX(5), RX(7)
RX(30) 4 **H** + O ===> **U** + V



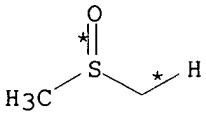
H



H

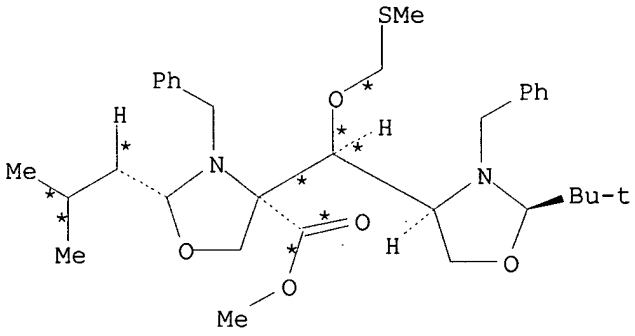


2 H

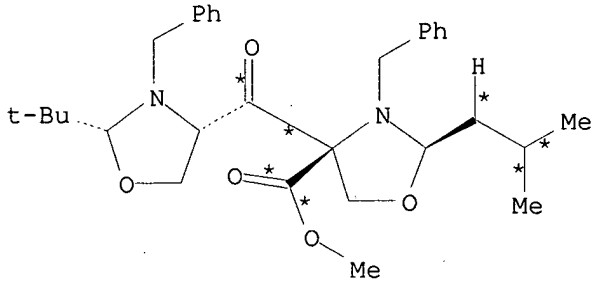


O

4
STEPS



U
YIELD 25%(50)



V
YIELD 25%(50)

RX(3) RCT H **145451-89-4**
RGT E 16940-66-2 NaBH4
PRO K 393867-18-0
SOL 67-56-1 MeOH, 109-99-9 THF

RX(4) RCT K 393867-18-0

STAGE(1)
RGT N 79-37-8 (COCl)2, O 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT D 121-44-8 Et3N

PRO M 393867-20-4
NTE Swern oxidn.

RX(5) RCT H **145451-89-4**

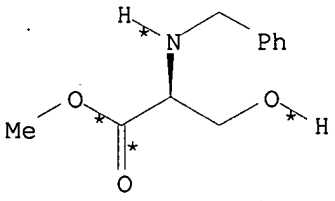
STAGE(1)
RGT R 4039-32-1 (Me3Si)2N.Li
SOL 109-99-9 THF

STAGE(2)
RCT M 393867-20-4

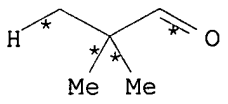
PRO Q 393867-22-6
NTE stereoselective, optimization study, optimized on base,additives,time

RX(7) RCT Q 393867-22-6, O 67-68-5
RGT W 108-24-7 Ac2O
PRO U **393867-28-2**, V 393867-30-6
SOL 64-19-7 AcOH

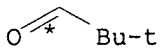
RX(39) OF 61 COMPOSED OF RX(2), RX(3), RX(4), RX(5), RX(7)
RX(39) 4 C + 4 G + 3 **H** + O ===> U + **V**



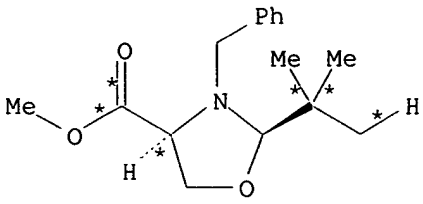
4 C



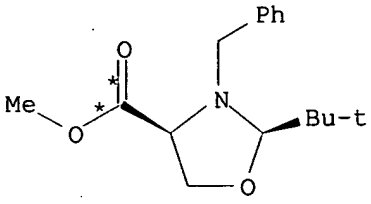
2 G



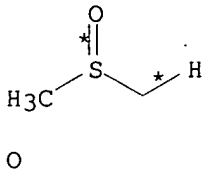
2 G



H

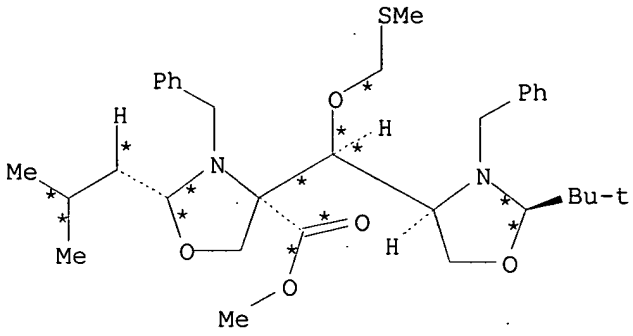


2 H

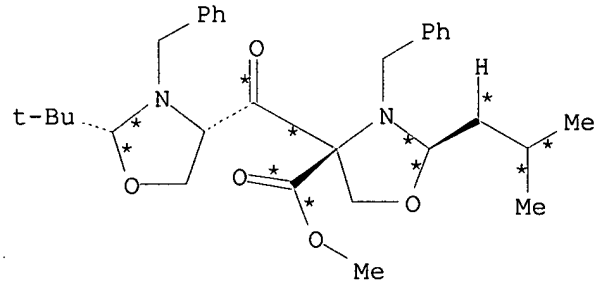


O

5
STEPS



U
YIELD 25%(50)



V
YIELD 25%(50)

RX(2) RCT C 123639-56-5, G 630-19-3
PRO H 145451-89-4
CAT 104-15-4 TsOH
SOL 108-88-3 PhMe
NTE stereoselective

RX(3) RCT H **145451-89-4**
RGT E 16940-66-2 NaBH4
PRO K 393867-18-0
SOL 67-56-1 MeOH, 109-99-9 THF

RX(4) RCT K 393867-18-0

STAGE(1)
RGT N 79-37-8 (COCl)2, O 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT D 121-44-8 Et3N

PRO M 393867-20-4
NTE Swern oxidn.

RX(5) RCT H **145451-89-4**

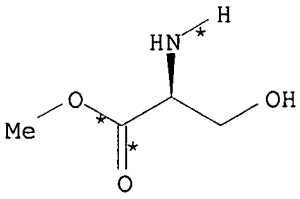
STAGE(1)
RGT R 4039-32-1 (Me3Si)2N.Li
SOL 109-99-9 THF

STAGE(2)
RCT M 393867-20-4

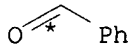
PRO Q 393867-22-6
NTE stereoselective, optimization study, optimized on base,additives,time

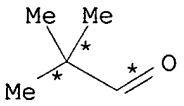
RX(7) RCT Q 393867-22-6, O 67-68-5
RGT W 108-24-7 Ac2O
PRO U 393867-28-2, V **393867-30-6**
SOL 64-19-7 AcOH

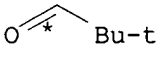
RX(44) OF 61 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(7)
RX(44) 4 A + 4 B + 4 G + 3 **H** + O ===> U + **V**



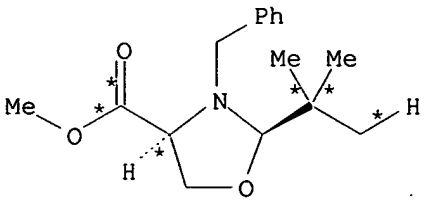
● HCl



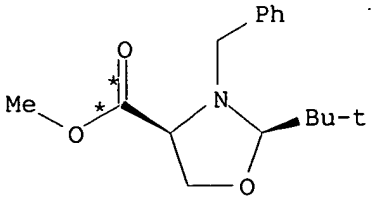




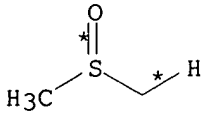
4 A 4 B 2 G 2 G



H

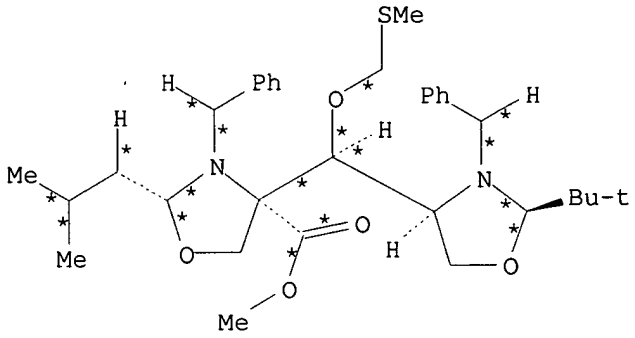


2 H

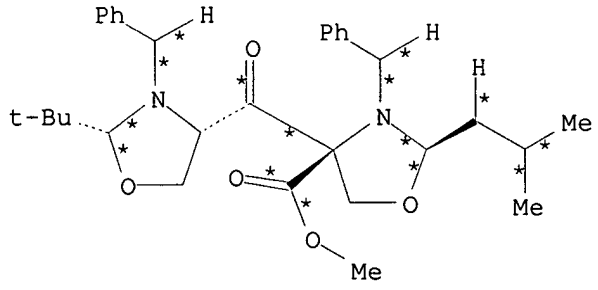


O

6
STEPS



U
YIELD 25%(50)



V
YIELD 25%(50)

RX(1) RCT A 5680-80-8, B 100-52-7

STAGE(1)

RGT D 121-44-8 Et3N
SOL 67-56-1 MeOH

STAGE(2)
RGT E 16940-66-2 NaBH4

PRO C 123639-56-5

RX(2) RCT C 123639-56-5, G 630-19-3
PRO H 145451-89-4
CAT 104-15-4 TsOH
SOL 108-88-3 PhMe
NTE stereoselective

RX(3) RCT H **145451-89-4**
RGT E 16940-66-2 NaBH4
PRO K 393867-18-0
SOL 67-56-1 MeOH, 109-99-9 THF

RX(4) RCT K 393867-18-0

STAGE(1)
RGT N 79-37-8 (COCl)2, O 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT D 121-44-8 Et3N

PRO M 393867-20-4
NTE Swern oxidn.

RX(5) RCT H **145451-89-4**

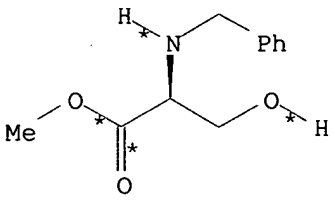
STAGE(1)
RGT R 4039-32-1 (Me3Si)2N.Li
SOL 109-99-9 THF

STAGE(2)
RCT M 393867-20-4

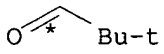
PRO Q 393867-22-6
NTE stereoselective, optimization study, optimized on base,additives,time

RX(7) RCT Q 393867-22-6, O 67-68-5
RGT W 108-24-7 Ac2O
PRO U 393867-28-2, V **393867-30-6**
SOL 64-19-7 AcOH

RX(50) OF 61 COMPOSED OF REACTION SEQUENCE RX(2), RX(5), RX(7)
AND REACTION SEQUENCE RX(3), RX(4), RX(5), RX(7)
...2 C + 2 G ===> H...
...3 **H** + O ===> **U** + V

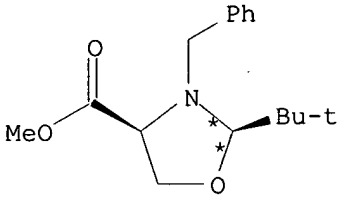


2 C



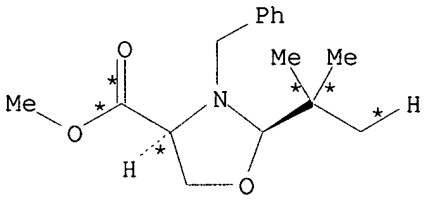
2 G

4 STEPS

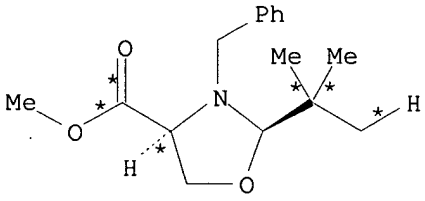


H

START NEXT REACTION SEQUENCE



H



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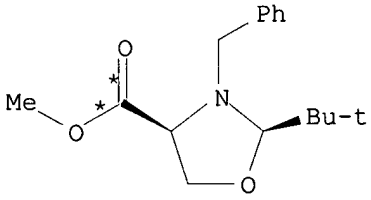

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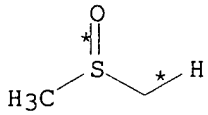
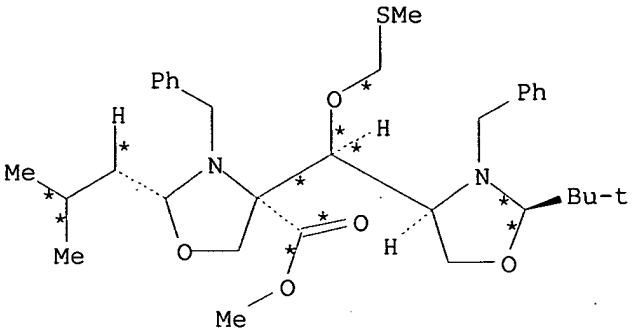
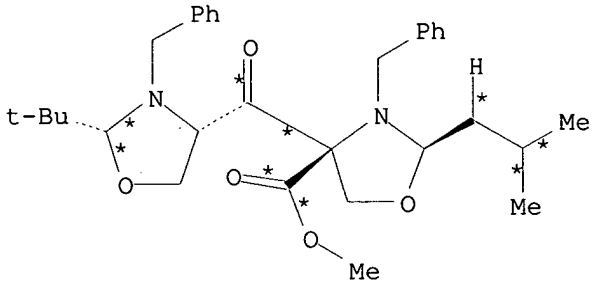


O

4 STEPS



U
YIELD 25%(50)



V
YIELD 25%(50)

RX(2) RCT C 123639-56-5, G 630-19-3
PRO H 145451-89-4
CAT 104-15-4 TsOH
SOL 108-88-3 PhMe
NTE stereoselective

RX(3) RCT H **145451-89-4**
RGT E 16940-66-2 NaBH4
PRO K 393867-18-0
SOL 67-56-1 MeOH, 109-99-9 THF

RX(4) RCT K 393867-18-0

STAGE(1)
RGT N 79-37-8 (COCl)2, O 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT D 121-44-8 Et3N

PRO M 393867-20-4
NTE Swern oxidn.

RX(5) RCT H **145451-89-4**

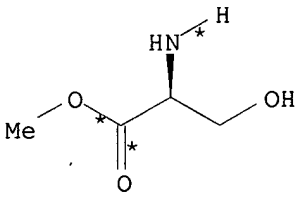
STAGE(1)
RGT R 4039-32-1 (Me3Si)2N.Li
SOL 109-99-9 THF

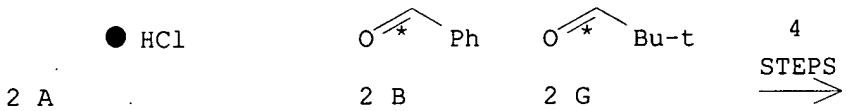
STAGE(2)
RCT M 393867-20-4

PRO Q 393867-22-6
NTE stereoselective, optimization study, optimized on base,additives,time

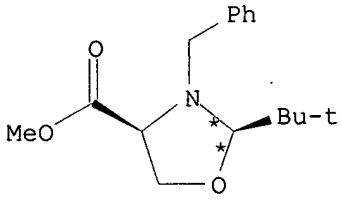
RX(7) RCT Q 393867-22-6, O 67-68-5
RGT W 108-24-7 Ac2O
PRO U **393867-28-2**, V 393867-30-6
SOL 64-19-7 AcOH

RX(51) OF 61 COMPOSED OF REACTION SEQUENCE RX(1), RX(2), RX(5), RX(7) AND REACTION SEQUENCE RX(3), RX(4), RX(5), RX(7)
...2 A + 2 B + 2 G ===> H...
...3 **H** + O ===> **U** + V



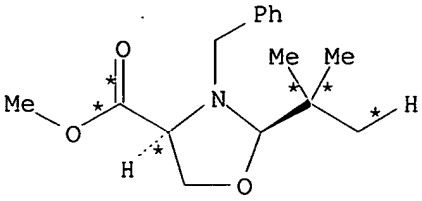


2 A 2 B 2 G



H

START NEXT REACTION SEQUENCE



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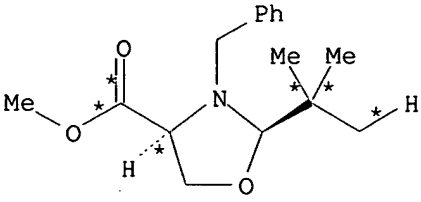

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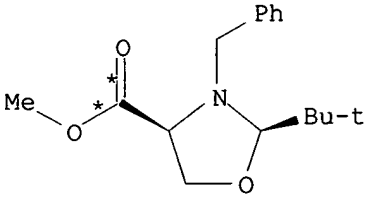

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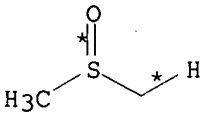
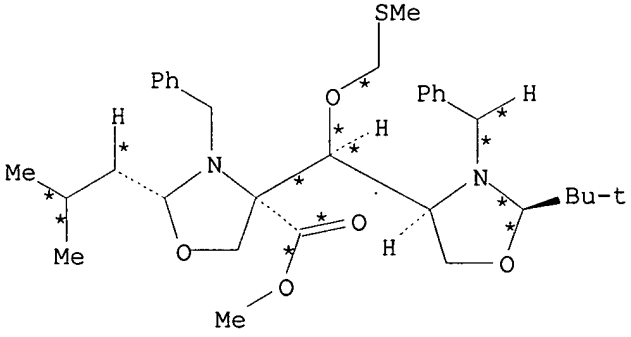
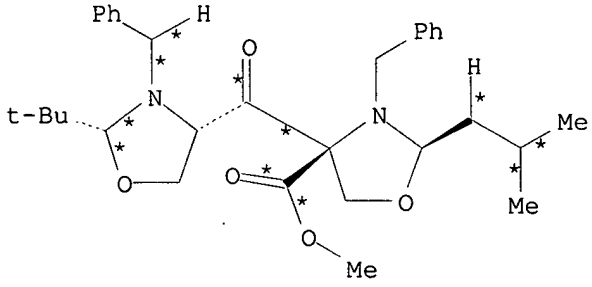


O

4
STEPS



U
YIELD 25%(50)



V
YIELD 25%(50)

RX(1) RCT A 5680-80-8, B 100-52-7

STAGE(1)
RGT D 121-44-8 Et3N
SOL 67-56-1 MeOH

STAGE(2)
RGT E 16940-66-2 NaBH4

PRO C 123639-56-5

RX(2) RCT C 123639-56-5, G 630-19-3
PRO H 145451-89-4
CAT 104-15-4 TsOH
SOL 108-88-3 PhMe
NTE stereoselective

RX(3) RCT H **145451-89-4**
RGT E 16940-66-2 NaBH4
PRO K 393867-18-0
SOL 67-56-1 MeOH, 109-99-9 THF

RX(4) RCT K 393867-18-0

STAGE(1)
RGT N 79-37-8 (COCl)2, O 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT D 121-44-8 Et3N

PRO M 393867-20-4
NTE Swern oxidn.

RX(5) RCT H **145451-89-4**

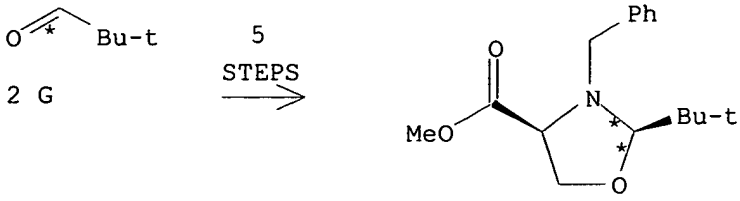
STAGE(1)
RGT R 4039-32-1 (Me3Si)2N.Li
SOL 109-99-9 THF

STAGE(2)
RCT M 393867-20-4

PRO Q 393867-22-6
NTE stereoselective, optimization study, optimized on base,additives,time

RX(7) RCT Q 393867-22-6, O 67-68-5
RGT W 108-24-7 Ac2O
PRO U **393867-28-2**, V 393867-30-6
SOL 64-19-7 AcOH

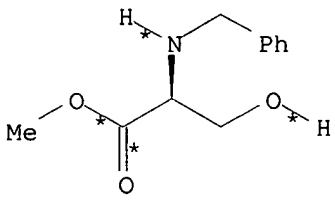
RX(53) OF 61 COMPOSED OF REACTION SEQUENCE RX(2), RX(5), RX(7)
AND REACTION SEQUENCE RX(2), RX(3), RX(4), RX(5), RX(7)
...3 C + 3 G ===> H...
...C + G + 2 **H** + O ===> U + **V**



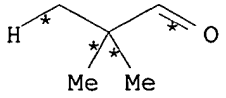
2 G

H

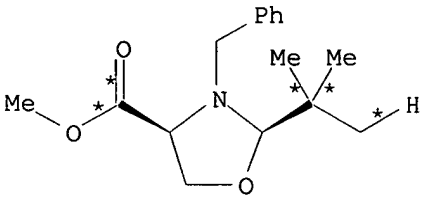
START NEXT REACTION SEQUENCE



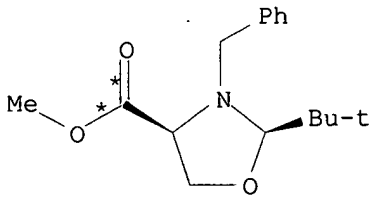
4 C



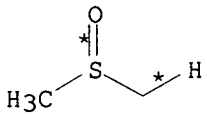
2 G



H

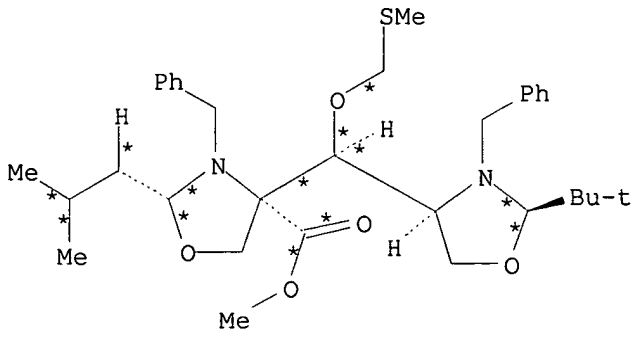


H

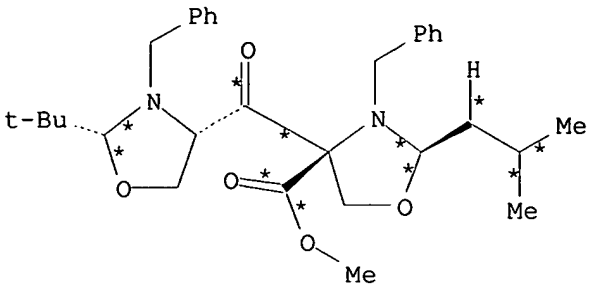


O

5
STEPS



U
YIELD 25%(50)



V
YIELD 25%(50)

RX(2) RCT C 123639-56-5, G 630-19-3
PRO H 145451-89-4
CAT 104-15-4 TsOH
SOL 108-88-3 PhMe
NTE stereoselective

RX(2) RCT C 123639-56-5, G 630-19-3
PRO H 145451-89-4
CAT 104-15-4 TsOH
SOL 108-88-3 PhMe
NTE stereoselective

RX(3) RCT H **145451-89-4**
RGT E 16940-66-2 NaBH4
PRO K 393867-18-0
SOL 67-56-1 MeOH, 109-99-9 THF

RX(4) RCT K 393867-18-0

STAGE(1)
RGT N 79-37-8 (COCl)2, O 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT D 121-44-8 Et3N

PRO M 393867-20-4
NTE Swern oxidn.

RX(5) RCT H **145451-89-4**

STAGE(1)
RGT R 4039-32-1 (Me3Si)2N.Li
SOL 109-99-9 THF

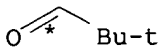
STAGE(2)
RCT M 393867-20-4

PRO Q 393867-22-6
NTE stereoselective, optimization study, optimized on base,additives,time

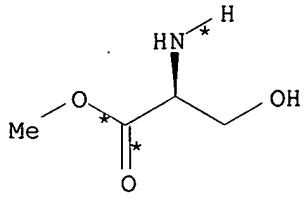
RX(7) RCT Q 393867-22-6, O 67-68-5

RGT W 108-24-7 Ac2O
PRO U 393867-28-2, V **393867-30-6**
SOL 64-19-7 AcOH

RX(54) OF 61 COMPOSED OF REACTION SEQUENCE RX(1), RX(2), RX(5), RX(7)
AND REACTION SEQUENCE RX(2), RX(3), RX(4), RX(5), RX(7)
...2 A + 2 B + 3 G ===> H...
...C + G + 2 **H** + O ===> U + **V**

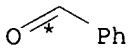


2 G



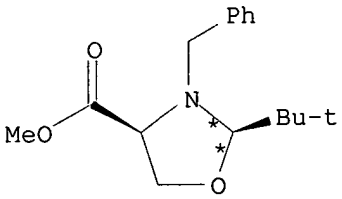
● HCl

2 A



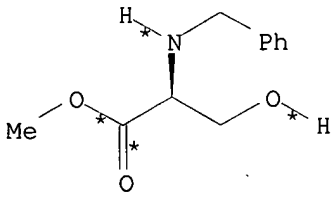
2 B

5 STEPS →

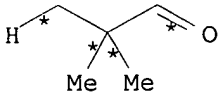


H

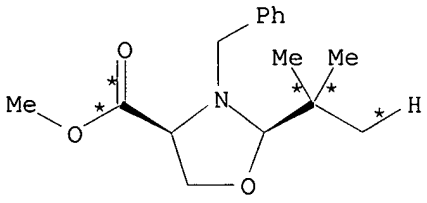
START NEXT REACTION SEQUENCE



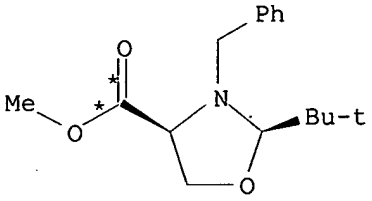
C



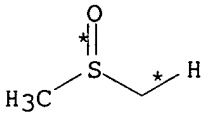
2 G



H

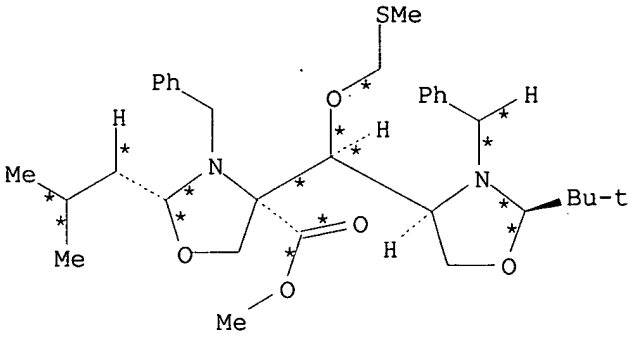


H

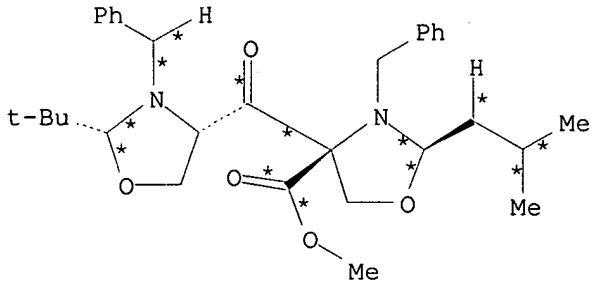


O

5 STEPS



U
YIELD 25%(50)



V
YIELD 25%(50)

RX(1) RCT A 5680-80-8, B 100-52-7

STAGE(1)
RGT D 121-44-8 Et3N
SOL 67-56-1 MeOH

STAGE(2)
RGT E 16940-66-2 NaBH4

PRO C 123639-56-5

RX(2) RCT C 123639-56-5, G 630-19-3
PRO H 145451-89-4
CAT 104-15-4 TsOH
SOL 108-88-3 PhMe
NTE stereoselective

RX(2) RCT C 123639-56-5, G 630-19-3
PRO H 145451-89-4
CAT 104-15-4 TsOH
SOL 108-88-3 PhMe
NTE stereoselective

RX(3) RCT H **145451-89-4**
RGT E 16940-66-2 NaBH4
PRO K 393867-18-0
SOL 67-56-1 MeOH, 109-99-9 THF

RX(4) RCT K 393867-18-0

STAGE(1)
RGT N 79-37-8 (COCl)2, O 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT D 121-44-8 Et3N

PRO M 393867-20-4
NTE Swern oxidn.

RX(5) RCT H **145451-89-4**

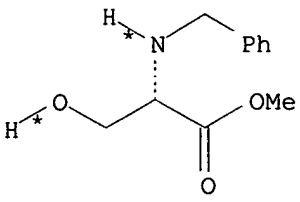
STAGE(1)
RGT R 4039-32-1 (Me3Si)2N.Li
SOL 109-99-9 THF

STAGE(2)
RCT M 393867-20-4

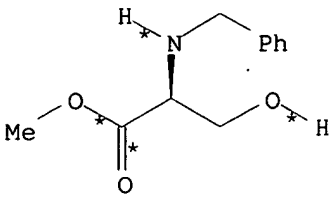
PRO Q 393867-22-6
NTE stereoselective, optimization study, optimized on base,additives,time

RX(7) RCT Q 393867-22-6, O 67-68-5
RGT W 108-24-7 Ac2O
PRO U 393867-28-2, V **393867-30-6**
SOL 64-19-7 AcOH

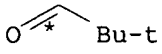
RX(56) OF 61 COMPOSED OF REACTION SEQUENCE RX(2), RX(5), RX(7)
AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(4), RX(5), RX(7)
...3 C + 3 G ===> H...
...2 A + 2 B + G + 2 **H** + O ===> U + **V**



C

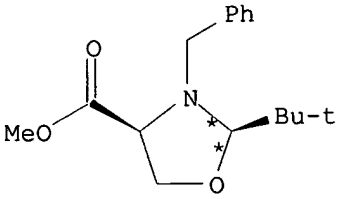


2 C



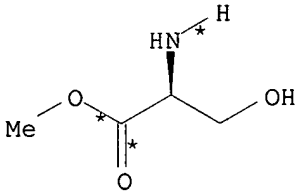
2 G

6 STEPS



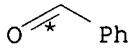
H

START NEXT REACTION SEQUENCE

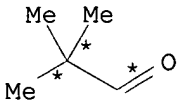


● HCl

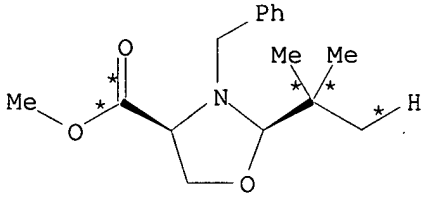
2 A



2 B



2 G



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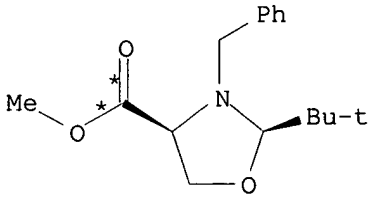

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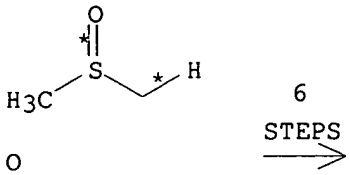

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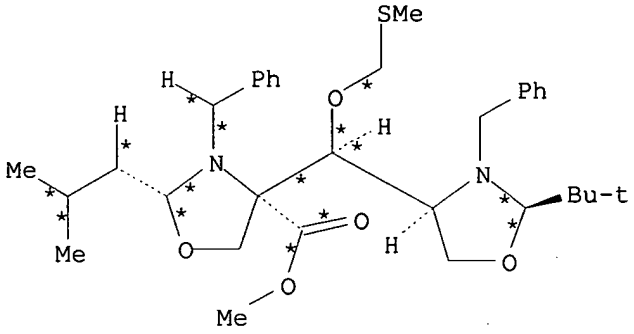
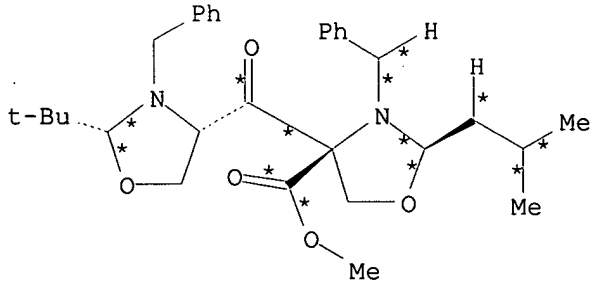


U
YIELD 25%(50)



V
YIELD 25%(50)

RX(2) RCT C 123639-56-5, G 630-19-3
PRO H 145451-89-4
CAT 104-15-4 TsOH
SOL 108-88-3 PhMe
NTE stereoselective

RX(1) RCT A 5680-80-8, B 100-52-7

STAGE(1)
RGT D 121-44-8 Et3N
SOL 67-56-1 MeOH

STAGE(2)
RGT E 16940-66-2 NaBH4

PRO C 123639-56-5

RX(2) RCT C 123639-56-5, G 630-19-3
PRO H 145451-89-4
CAT 104-15-4 TsOH
SOL 108-88-3 PhMe
NTE stereoselective

RX(3) RCT H **145451-89-4**
RGT E 16940-66-2 NaBH4
PRO K 393867-18-0
SOL 67-56-1 MeOH, 109-99-9 THF

RX(4) RCT K 393867-18-0

STAGE(1)
RGT N 79-37-8 (COCl)2, O 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT D 121-44-8 Et3N

PRO M 393867-20-4
NTE Swern oxidn.

RX(5) RCT H **145451-89-4**

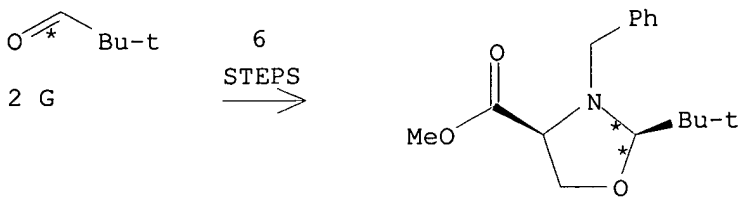
STAGE(1)
RGT R 4039-32-1 (Me3Si)2N.Li
SOL 109-99-9 THF

STAGE(2)
RCT M 393867-20-4

PRO Q 393867-22-6
NTE stereoselective, optimization study, optimized on base,additives,time

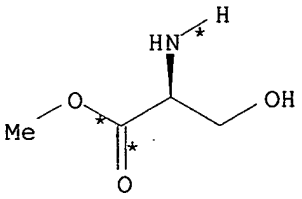
RX(7) RCT Q 393867-22-6, O 67-68-5
RGT W 108-24-7 Ac2O
PRO U 393867-28-2, V **393867-30-6**
SOL 64-19-7 AcOH

RX(57) OF 61 COMPOSED OF REACTION SEQUENCE RX(1), RX(2), RX(5), RX(7)
AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(4), RX(5), RX(7)
...3 A + 3 B + 3 G ===> H...
...A + B + G + 2 **H** + O ===> U + **V**



H

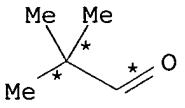
START NEXT REACTION SEQUENCE



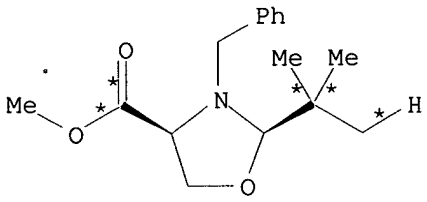
● HCl

4 A

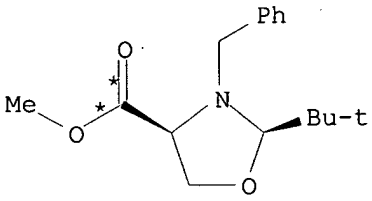
4 B



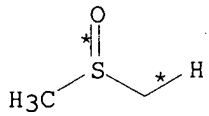
2 G



H

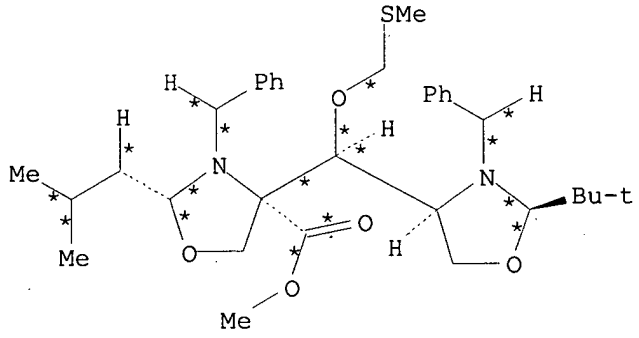


H

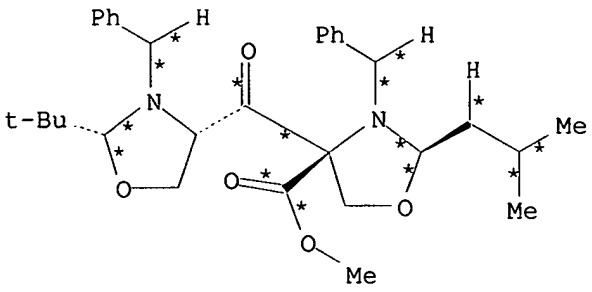


O

6
STEPS



U
YIELD 25%(50)



V
YIELD 25%(50)

RX(1) RCT A 5680-80-8, B 100-52-7

STAGE(1)
RGT D 121-44-8 Et3N
SOL 67-56-1 MeOH

STAGE(2)
RGT E 16940-66-2 NaBH4

PRO C 123639-56-5

RX(2) RCT C 123639-56-5, G 630-19-3
PRO H 145451-89-4
CAT 104-15-4 TsOH
SOL 108-88-3 PhMe
NTE stereoselective

RX(1) RCT A 5680-80-8, B 100-52-7

STAGE(1)
RGT D 121-44-8 Et3N
SOL 67-56-1 MeOH

STAGE(2)
RGT E 16940-66-2 NaBH4

PRO C 123639-56-5

RX(2) RCT C 123639-56-5, G 630-19-3
PRO H 145451-89-4
CAT 104-15-4 TsOH
SOL 108-88-3 PhMe
NTE stereoselective

RX(3) RCT H **145451-89-4**
RGT E 16940-66-2 NaBH4
PRO K 393867-18-0
SOL 67-56-1 MeOH, 109-99-9 THF

RX(4) RCT K 393867-18-0

STAGE(1)
RGT N 79-37-8 (COCl)2, O 67-68-5 DMSO

SOL 75-09-2 CH2Cl2

STAGE(2)
RGT D 121-44-8 Et3N

PRO M 393867-20-4
NTE Swern oxidn.

RX(5) RCT H **145451-89-4**

STAGE(1)
RGT R 4039-32-1 (Me3Si)2N.Li
SOL 109-99-9 THF

STAGE(2)
RCT M 393867-20-4

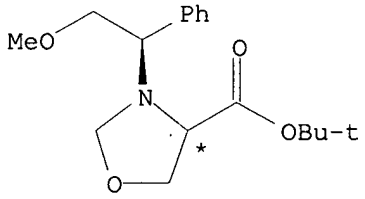
PRO Q 393867-22-6
NTE stereoselective, optimization study, optimized on base,additives,time

RX(7) RCT Q 393867-22-6, O 67-68-5
RGT W 108-24-7 Ac2O
PRO U 393867-28-2, V **393867-30-6**
SOL 64-19-7 AcOH

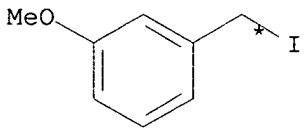
L3 ANSWER 9 OF 17 CASREACT COPYRIGHT 2005 ACS on STN

9

RX(1) OF 13 **A** + B ===> **C**...

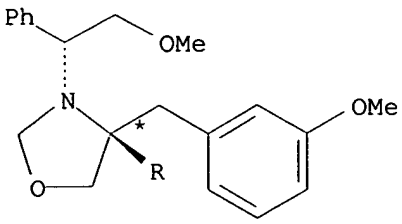


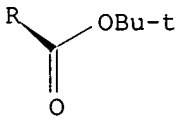
A



B

(1) →





C
YIELD 64%

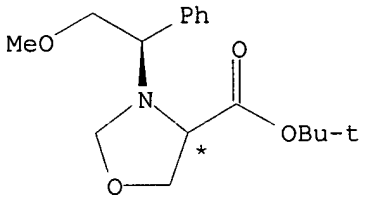
RX(1) RCT A **271771-97-2**

STAGE(1)
RGT D 40949-94-8 K [N(SiMe3)2]
SOL 109-99-9 THF

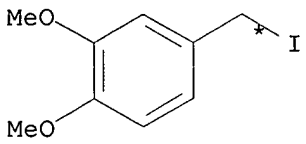
STAGE(2)
RCT B 90110-63-7

PRO C **342043-15-6**
NTE stereoselective

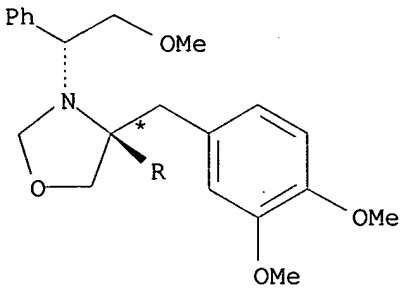
RX(2) OF 13 **A** + F ===> **G**...

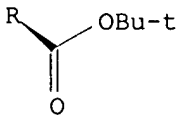


A



F





G
YIELD 74%

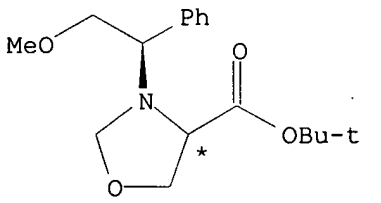
RX(2) RCT A **271771-97-2**

STAGE(1)
RGT D 40949-94-8 K [N(SiMe3)2]
SOL 109-99-9 THF

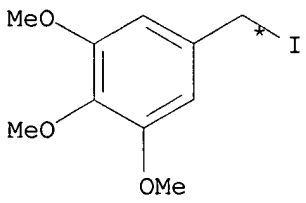
STAGE(2)
RCT F 76950-76-0

PRO G **342043-17-8**
NTE stereoselective

RX(3) OF 13 **A** + H ===> **I**...

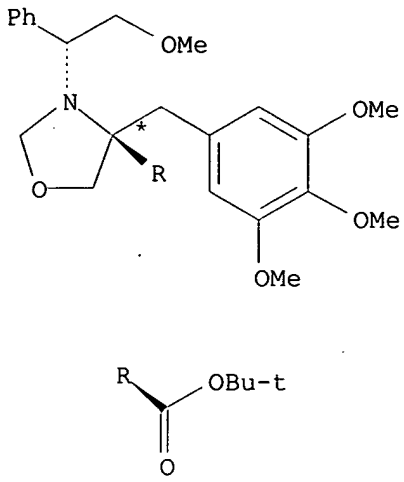


A



H

(3) →



I
YIELD 50%

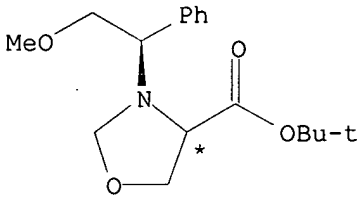
RX(3) RCT A **271771-97-2**

STAGE(1)
RGT D 40949-94-8 K [N(SiMe3)2]
SOL 109-99-9 THF

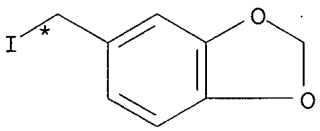
STAGE(2)
RCT H 18111-18-7

PRO I **342043-19-0**
NTE stereoselective

RX(4) OF 13 **A** + J ===> **K**...

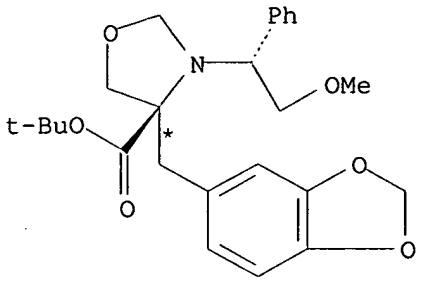


A



J

(4) →



K
YIELD 65%

RX(4) RCT A **271771-97-2**

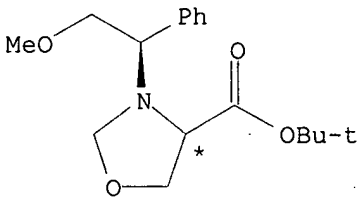
STAGE(1)
RGT D 40949-94-8 K [N(SiMe3)2]
SOL 109-99-9 THF

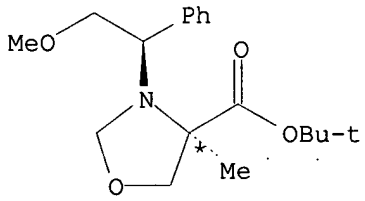
STAGE(2)
RCT J 157766-09-1

PRO K **342043-21-4**
NTE stereoselective

L3 ANSWER 10 OF 17 CASREACT COPYRIGHT 2005 ACS on STN

RX(3) OF 48 ...**G** + I ===> **J**...





G I J

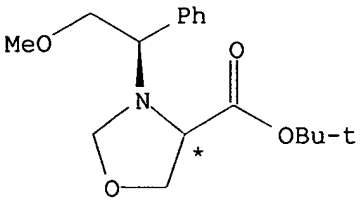
RX(3) RCT G **271771-97-2**

STAGE(1)
RGT K 40949-94-8 K [N(SiMe3)2]
SOL 109-99-9 THF

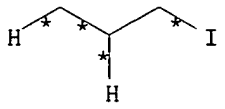
STAGE(2)
RCT I 74-88-4

PRO J **271771-98-3**
NTE stereoselective key step; (95% d.e.)

RX(4) OF 48 ...**G** + M ===> **N**...

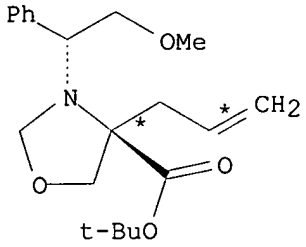


G



M

(4) →



N
YIELD 97%

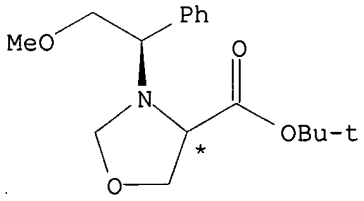
RX(4) RCT G **271771-97-2**

STAGE(1)
RGT K 40949-94-8 K [N(SiMe3)2]
SOL 109-99-9 THF

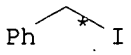
STAGE(2)
RCT M 107-08-4

PRO N **271772-00-0**
NTE stereoselective key step; (86% d.e.)

RX(5) OF 48 ...**G** + O ===> **P**...

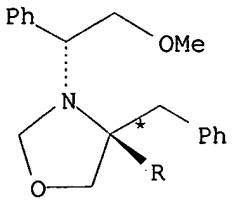


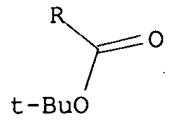
G



O

(5) →





P

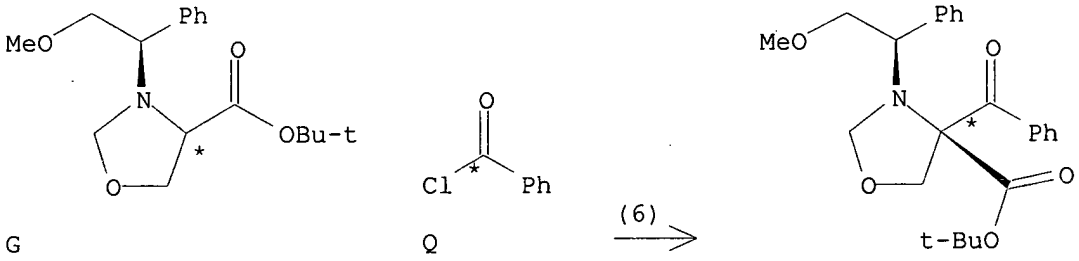
RX(5) RCT G **271771-97-2**

STAGE(1)
RGT K 40949-94-8 K [N(SiMe3)2]
SOL 109-99-9 THF

STAGE(2)
RCT O 620-05-3

PRO P **271772-01-1**
NTE stereoselective key step (88% d.e.)

RX(6) OF 48 ...**G** + Q ===> **R**



G Q R

YIELD 73%

RX(6) RCT G **271771-97-2**

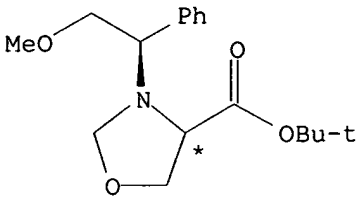
STAGE(1)
RGT K 40949-94-8 K [N(SiMe3)2]
SOL 109-99-9 THF

STAGE(2)
RCT Q 98-88-4

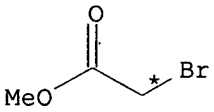
PRO R **271772-02-2**

NTE stereoselective key step (81% d.e.)

RX(7) OF 48 ...**G** + S ===> **T**...

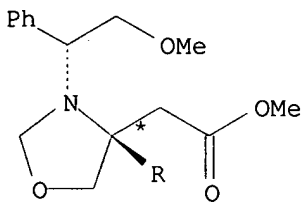


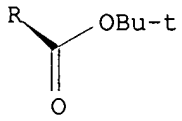
G



S

(7) ⟶





T

RX(7) RCT G **271771-97-2**

K HMDA
THF

STAGE(1)
RGT K 40949-94-8 K [N(SiMe3)2]
SOL 109-99-9 THF

STAGE(2)
RCT S 96-32-2

PRO T **271772-03-3**
NTE stereoselective key step (95% d.e.)

L3 ANSWER 11 OF 17 CASREACT COPYRIGHT 2005 ACS on STN

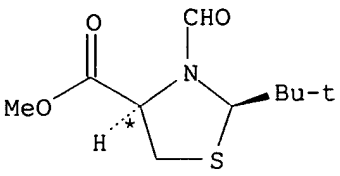
RX(3) OF 6 ...**C** + H ===> **D**...

11

Tet Lett

-78°C

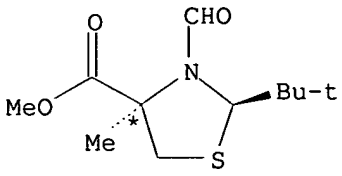
X



C

H

(3) →



D
YIELD 56%

RX(3) RCT C **104654-63-9**

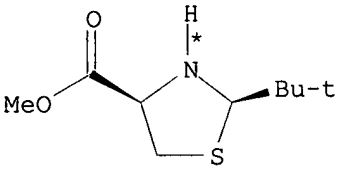
STAGE(1)
RGT I 4111-54-0 LiN(Pr-i)2, J 7226-23-5 DMPU
SOL 109-99-9 THF

LDA THF DMPU

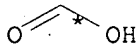
STAGE(2)
RCT H 74-88-4
SOL 109-99-9 THF

PRO D **148692-18-6**
NTE Stereoselective/key step

RX(4) OF 6 COMPOSED OF RX(1), RX(3)
RX(4) **A** + B + H ===> **D**



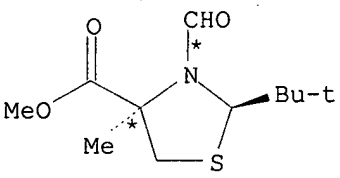
A



B

H

2 STEPS →



D
YIELD 56%

RX(1) RCT A **113234-78-9**, B 64-18-6
PRO C 104654-63-9
SOL 64-18-6 HCO2H

RX(3) RCT C 104654-63-9

STAGE(1)

RGT I 4111-54-0 LiN(Pr-i)2, J 7226-23-5 DMPU
SOL 109-99-9 THF

CDA DMPU
THF

STAGE(2)
RCT H 74-88-4
SOL 109-99-9 THF

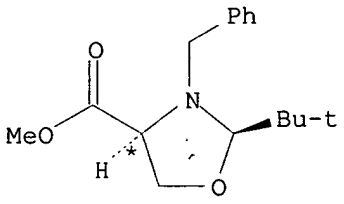
PRO D **148692-18-6**
NTE Stereoselective/key step

L3 ANSWER 12 OF 17 CASREACT COPYRIGHT 2005 ACS on STN

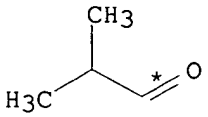
12

RX(2) OF 36 **G** + H ===> **I**...

JACS
-78°C X

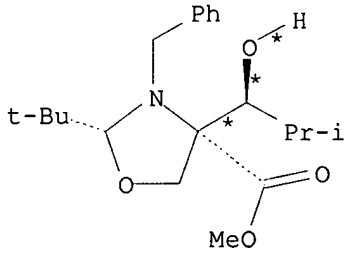


G



H

(2) →



I
YIELD 51%

RX(2) RCT G **145451-89-4**

LiBr
LDA

STAGE(1)
RCT J 7550-35-8 LiBr, K 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

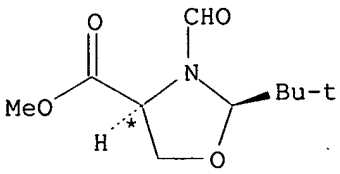
STAGE(2)
RCT H 78-84-2
SOL 109-99-9 THF

PRO I **145451-90-7**
NTE stereoselective; key step

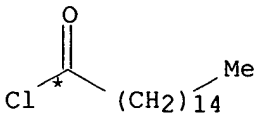
L3 ANSWER 13 OF 17 CASREACT COPYRIGHT 2005 ACS on STN

13

RX(1) OF 7 **A** + B ===> **C**...

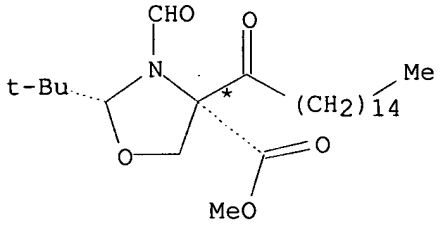


A



B

(1) →



C
YIELD 60%

RX(1) RCT A **93250-91-0**

STAGE(1)
RGT D 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF, 110-54-3 Hexane

BASE LDA / THF / Hex

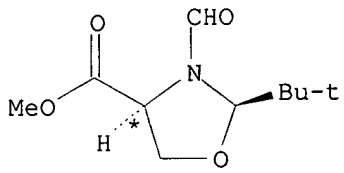
STAGE(2)
E^+ → RCT B 112-67-4
SOL 109-99-9 THF, 110-54-3 Hexane

PRO C **131148-72-6**
NTE key step

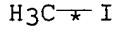
14

L3 ANSWER 14 OF 17 CASREACT COPYRIGHT 2005 ACS on STN

RX(33) OF 126 ...**BZ** + AL ===> **CE**...

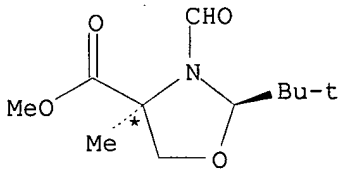


BZ



AL

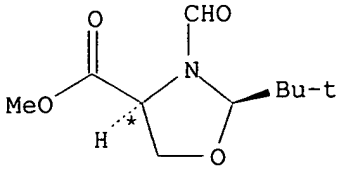
(33) →



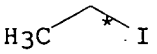
CE
YIELD 68%

RX(33) RCT BZ **93250-91-0**, AL 74-88-4
RGT H 4111-54-0 LiN(Pr-i)2
PRO CE **93250-94-3**
SOL 109-99-9 THF, 1608-26-0 P(NMe2)3

RX(34) OF 126 ...**BZ** + AO ===> **CF**

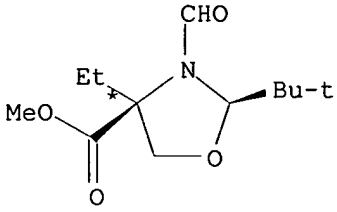


BZ



AO

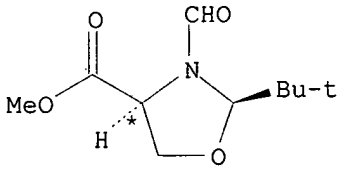
(34)



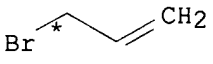
CF
YIELD 53%

RX(34) RCT BZ **93250-91-0**, AO 75-03-6
RGT H 4111-54-0 LiN(Pr-i)2
PRO CF **93250-95-4**
SOL 109-99-9 THF, 7226-23-5 DMPU

RX(35) OF 126 ...**BZ** + O ===> **CG**

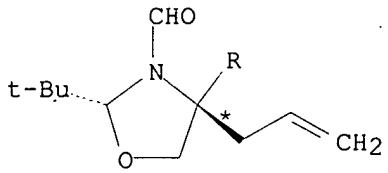


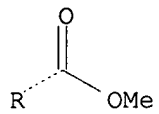
BZ



O

(35)



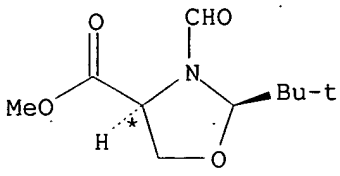


CG
YIELD 57%

RX(35) RCT BZ **93250-91-0**, O 106-95-6
RGT H 4111-54-0 LiN(Pr-i)2
PRO CG **93250-96-5**

SOL 109-99-9 THF, 1608-26-0 P(NMe2)3

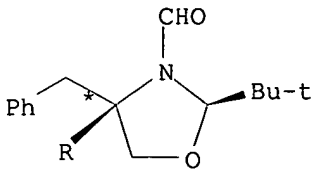
RX(36) OF 126 ...**BZ** + X ===> **CH**

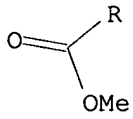


BZ

X

(36)



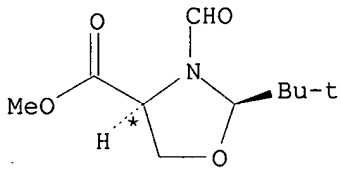


CH
YIELD 52%

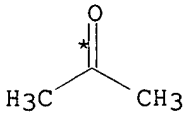
RX(36) RCT BZ **93250-91-0**, X 100-39-0
RGT H 4111-54-0 LiN(Pr-i)2
PRO CH **93250-97-6**
SOL 109-99-9 THF, 7226-23-5 DMPU

LDA / THF / DMPU

RX(37) OF 126 ...**BZ** + AY ===> **CI**

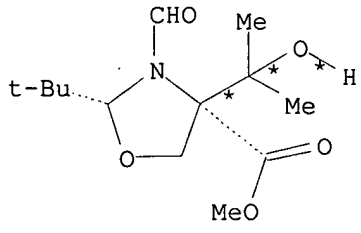


BZ



AY

(37)

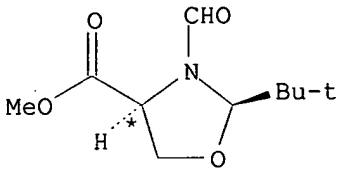


CI
YIELD 58%

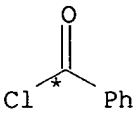
RX(37) RCT BZ **93250-91-0**, AY 67-64-1
RGT H 4111-54-0 LiN(Pr-i)2

PRO CI **93250-98-7**
SOL 109-99-9 THF

RX(38) OF 126 ...**BZ** + BJ ===> **CJ**

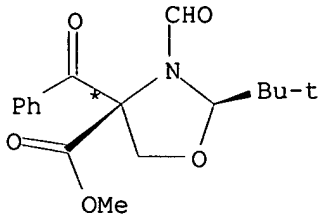


BZ



BJ

(38)

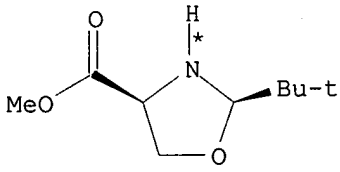


CJ
YIELD 70%

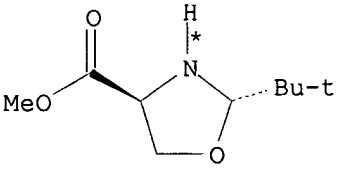
RX(38) RCT BZ **93250-91-0**, BJ 98-88-4
RGT H 4111-54-0 LiN(Pr-i)2
PRO CJ **114041-66-6**
SOL 109-99-9 THF

LDA / THF

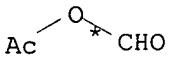
RX(69) OF 126 COMPOSED OF RX(31), RX(33)
RX(69) **BU** + BV + 2 BY + AL ===> **CE**



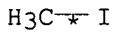
BU



BV

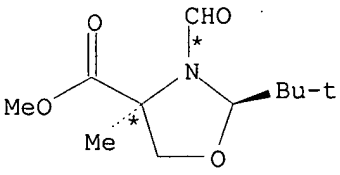


2 BY



AL

2 STEPS



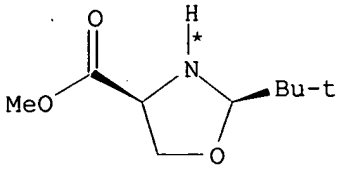
CE
YIELD 68%

RX(31) RCT BU **93250-89-6**, BV 93250-90-9, BY 2258-42-6
PRO BZ 93250-91-0, CA 93250-92-1
SOL 60-29-7 Et2O

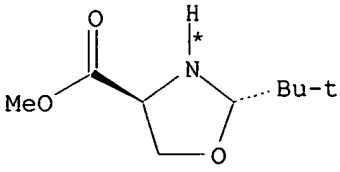
RX(33) RCT BZ 93250-91-0, AL 74-88-4
RGT H 4111-54-0 LiN(Pr-i)2
PRO CE **93250-94-3**
SOL 109-99-9 THF, 1608-26-0 P(NMe2)3

LDA / THF

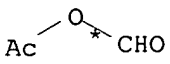
RX(70) OF 126 COMPOSED OF RX(31), RX(34)
RX(70) **BU** + BV + 2 BY + AO ===> **CF**



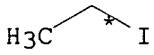
BU



BV

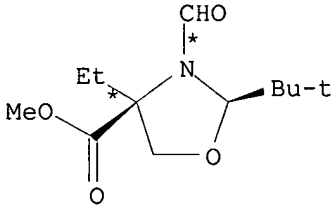


2 BY



AO

2 STEPS



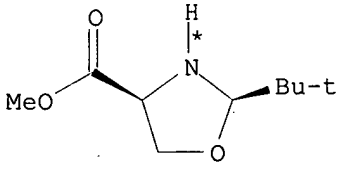
CF
YIELD 53%

RX(31) RCT BU **93250-89-6**, BV 93250-90-9, BY 2258-42-6
PRO BZ 93250-91-0, CA 93250-92-1
SOL 60-29-7 Et2O

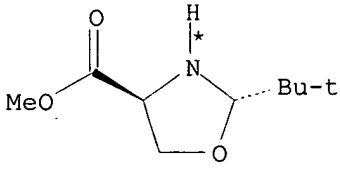
RX(34) RCT BZ 93250-91-0, AO 75-03-6
RGT H 4111-54-0 LiN(Pr-i)2
PRO CF **93250-95-4**
SOL 109-99-9 THF, 7226-23-5 DMPU

LDA / THF DMPU

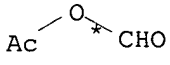
RX(71) OF 126 COMPOSED OF RX(31), RX(35)
RX(71) **BU** + BV + 2 BY + O ===> **CG**



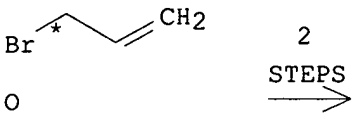
BU



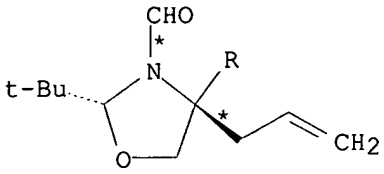
BV

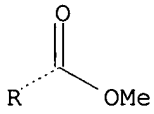


2 BY



2 STEPS



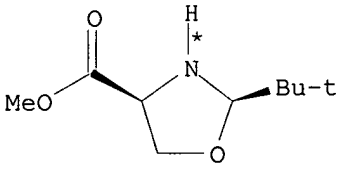


CG
YIELD 57%

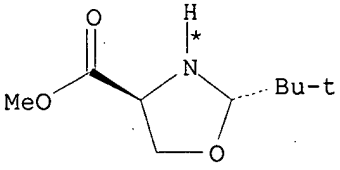
RX(31) RCT BU **93250-89-6**, BV 93250-90-9, BY 2258-42-6
PRO BZ 93250-91-0, CA 93250-92-1
SOL 60-29-7 Et2O

RX(35) RCT BZ 93250-91-0, O 106-95-6
RGT H 4111-54-0 LiN(Pr-i)2 LDA / THF
PRO CG **93250-96-5**
SOL 109-99-9 THF, 1608-26-0 P(NMe2)3

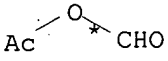
RX(72) OF 126 COMPOSED OF RX(31), RX(36)
RX(72) **BU** + BV + 2 BY + X ===> **CH**



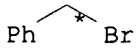
BU



BV

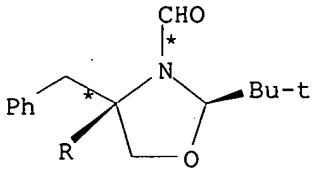


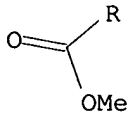
2 BY



2 STEPS

X





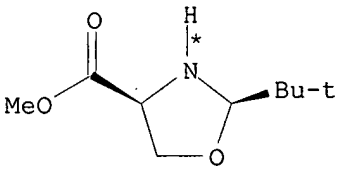
CH
YIELD 52%

RX(31) RCT BU **93250-89-6**, BV 93250-90-9, BY 2258-42-6
PRO BZ 93250-91-0, CA 93250-92-1
SOL 60-29-7 Et2O

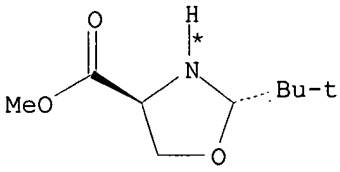
RX(36) RCT BZ 93250-91-0, X 100-39-0
RGT H 4111-54-0 LiN(Pr-i)2
PRO CH **93250-97-6**
SOL 109-99-9 THF, 7226-23-5 DMPU

LDA / THF DMPU

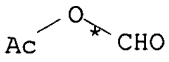
RX(73) OF 126 COMPOSED OF RX(31), RX(37)
RX(73) **BU** + BV + 2 BY + AY ===> **CI**



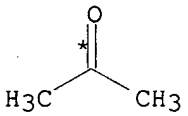
BU



BV

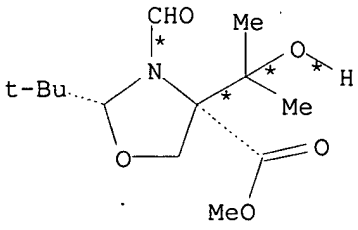


2 BY



AY

2 STEPS



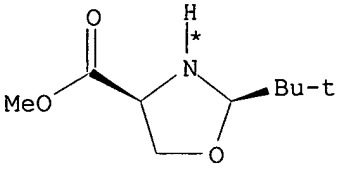
CI
YIELD 58%

RX(31) RCT BU **93250-89-6**, BV 93250-90-9, BY 2258-42-6
PRO BZ 93250-91-0, CA 93250-92-1

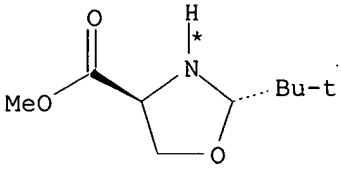
SOL 60-29-7 Et2O

RX(37) RCT BZ 93250-91-0, AY 67-64-1
RGT H 4111-54-0 LiN(Pr-i)2 LDA / THF
PRO CI **93250-98-7**.
SOL 109-99-9 THF

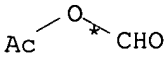
RX(74) OF 126 COMPOSED OF RX(31), RX(38)
RX(74) **BU** + BV + 2 BY + BJ ===> **CJ**



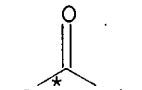
BU



BV

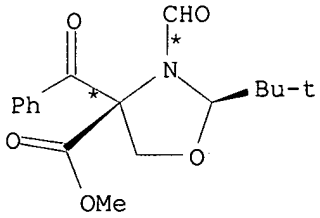


2 BY



BJ

2 STEPS



CJ
YIELD 70%

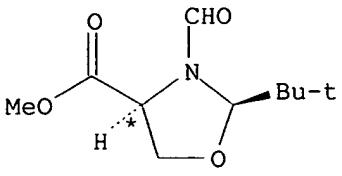
RX(31) RCT BU **93250-89-6**, BV 93250-90-9, BY 2258-42-6
PRO BZ 93250-91-0, CA 93250-92-1
SOL 60-29-7 Et2O

RX(38) RCT BZ 93250-91-0, BJ 98-88-4
RGT H 4111-54-0 LiN(Pr-i)2
PRO CJ **114041-66-6**
SOL 109-99-9 THF

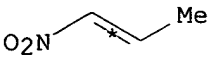
15

L3 ANSWER 15 OF 17 CASREACT COPYRIGHT 2005 ACS on STN

RX(11) OF 51 **Y** + B ===> **Z**

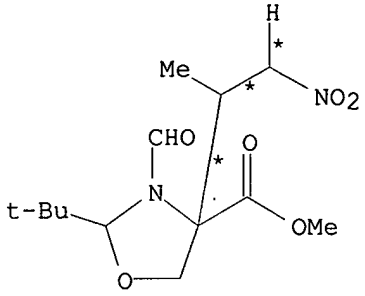


Y



B

(11) →



Z

RX(11) RCT Y **93250-91-0**

STAGE(1)
RGT D 4111-54-0 LiN(Pr-i)2
SOL 109-99-9 THF

STAGE(2)
RCT B 17082-05-2
SOL 109-99-9 THF

STAGE(3)
RGT E 64-19-7 AcOH
SOL 109-99-9 THF

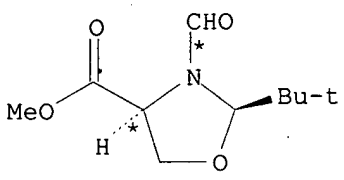
PRO Z **104194-12-9**

L3 ANSWER 16 OF 17 CASREACT COPYRIGHT 2005 ACS on STN

16

-78 °C

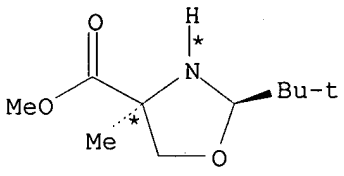
RX(1) OF 1 **A** + B ===> **C**



A

B

(1) →



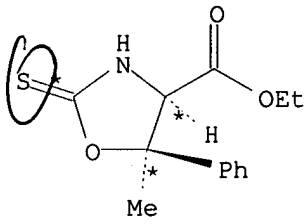
C
YIELD 68%

RX(1) RCT A **93250-91-0**, B 74-88-4
RGT D 4111-54-0 LiN(Pr-i)2
PRO C **521310-08-7**
SOL 109-99-9 THF, 1608-26-0 P(NMe2)3
NTE Classification: C-Methylation; Deformylation; Diastereoselective; # Conditions: LDA THF; dry ice bath; MeI HMPT

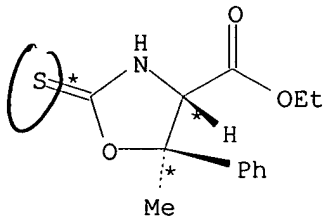
L3 ANSWER 17 OF 17 CASREACT COPYRIGHT 2005 ACS on STN

17

RX(23) OF 41 ...**AN** + N ===> 2 **AO**

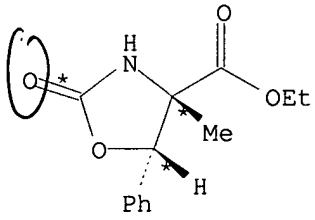


AN

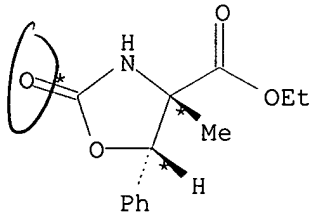


N

(23)



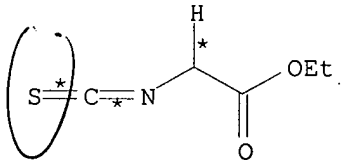
AO
YIELD 96%



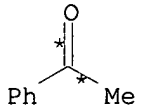
AO
YIELD 96%

RX(23) RCT AN **61079-00-3**, N 61079-01-4
PRO AO **61079-08-1**

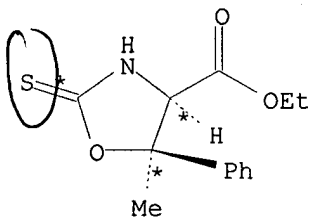
RX(33) OF 41 COMPOSED OF RX(7), RX(23)
RX(33) A + M + **AN** ===> 2 **AO**



A



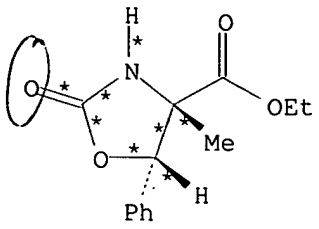
M



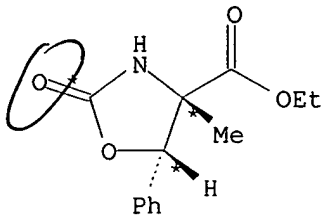
AN

2 STEPS

cyclization



AO
YIELD 96%



AO
YIELD 96%

RX(7) RCT A 24066-82-8, M 98-86-2
RGT O 7646-69-7 NaH
PRO N 61079-01-4

RX(23) RCT AN **61079-00-3**, N 61079-01-4
PRO AO **61079-08-1**

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	181.88	182.09

STN INTERNATIONAL LOGOFF AT 16:12:18 ON 15 NOV 2005